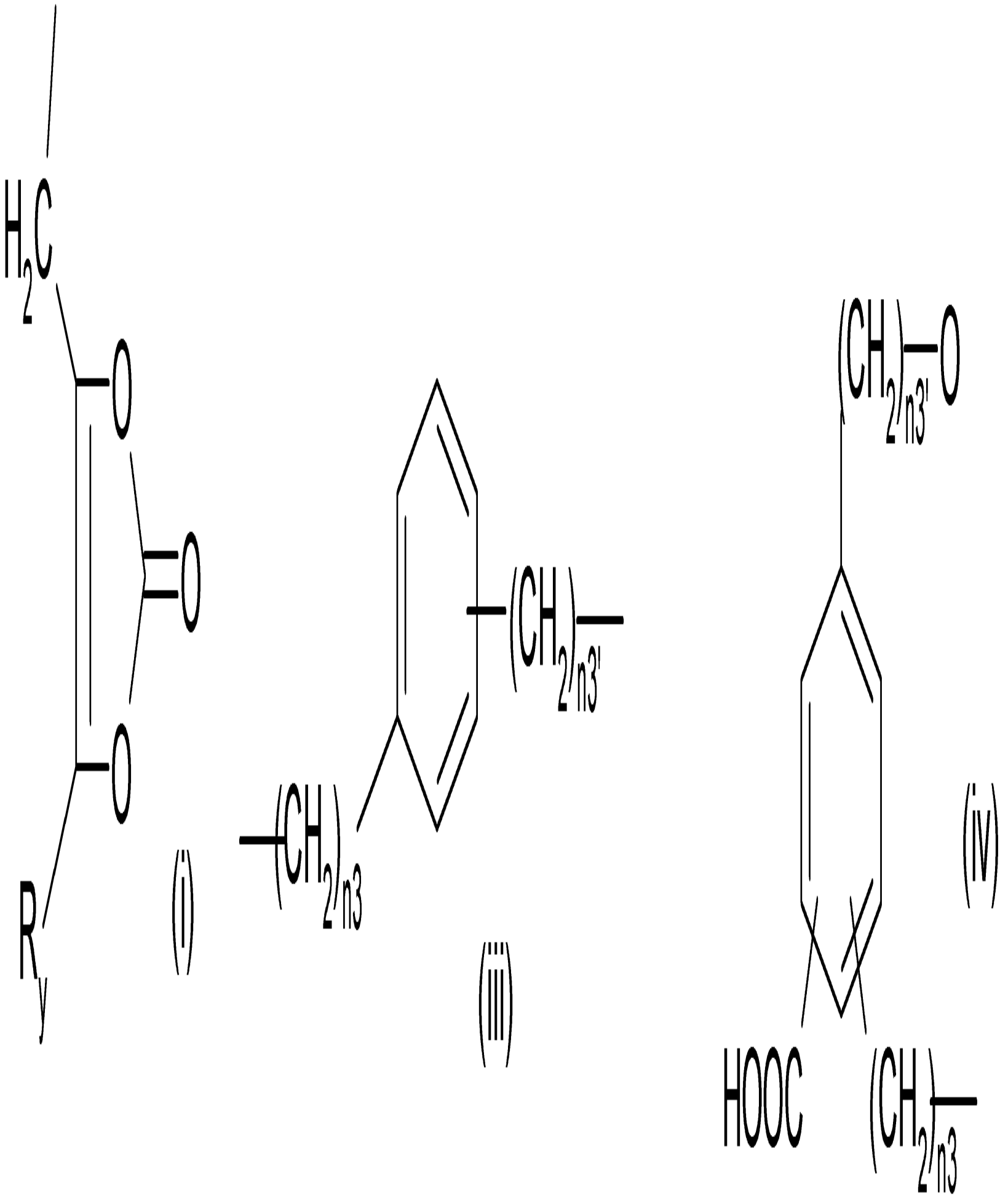
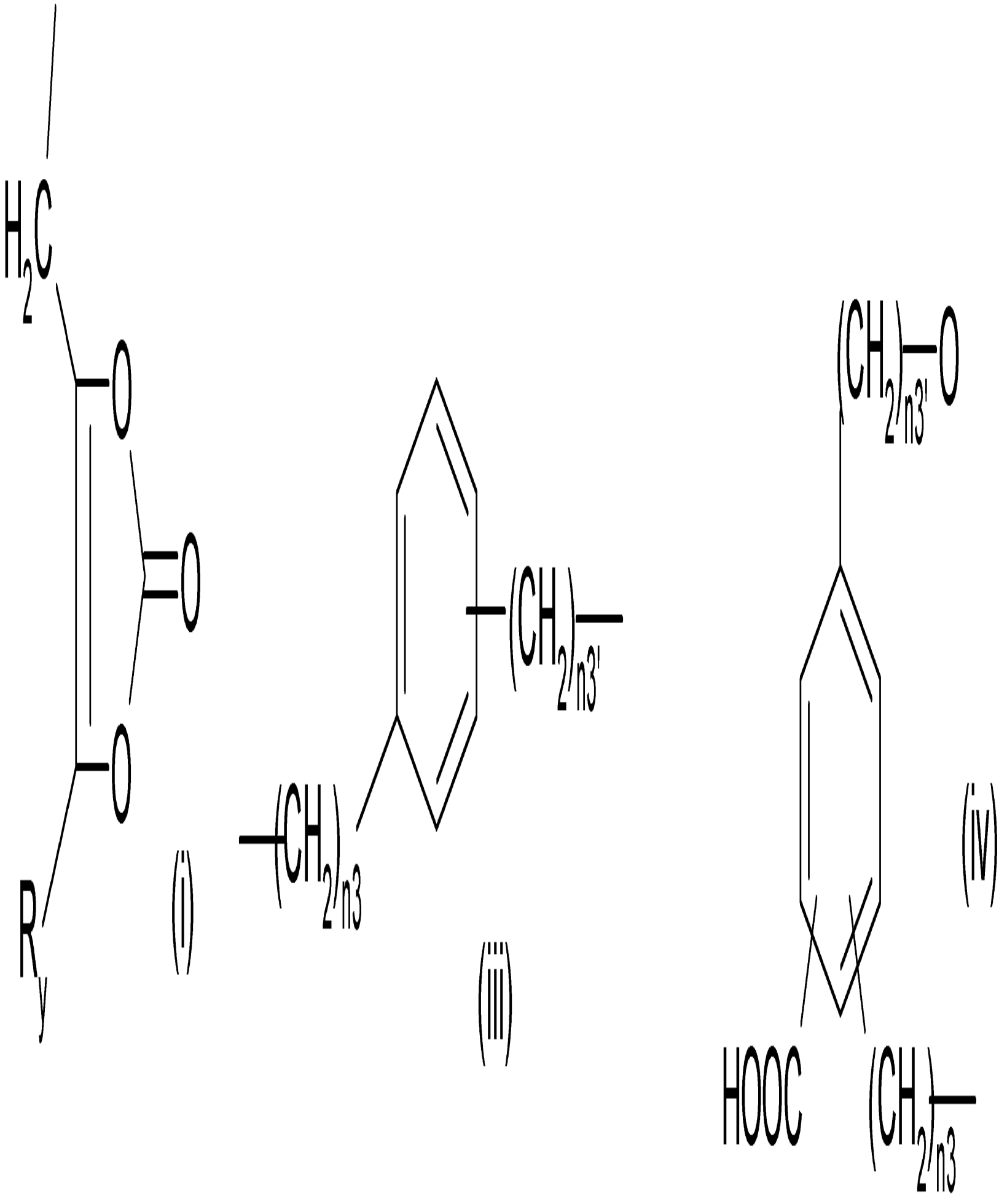

H2C
O
O
O
Ry
(ii)
(CH2)n3
(CH2)n3'
(iii)
(CH2)n3'—O
HOOC
(CH2)n3
(iv)


H2C
O
O
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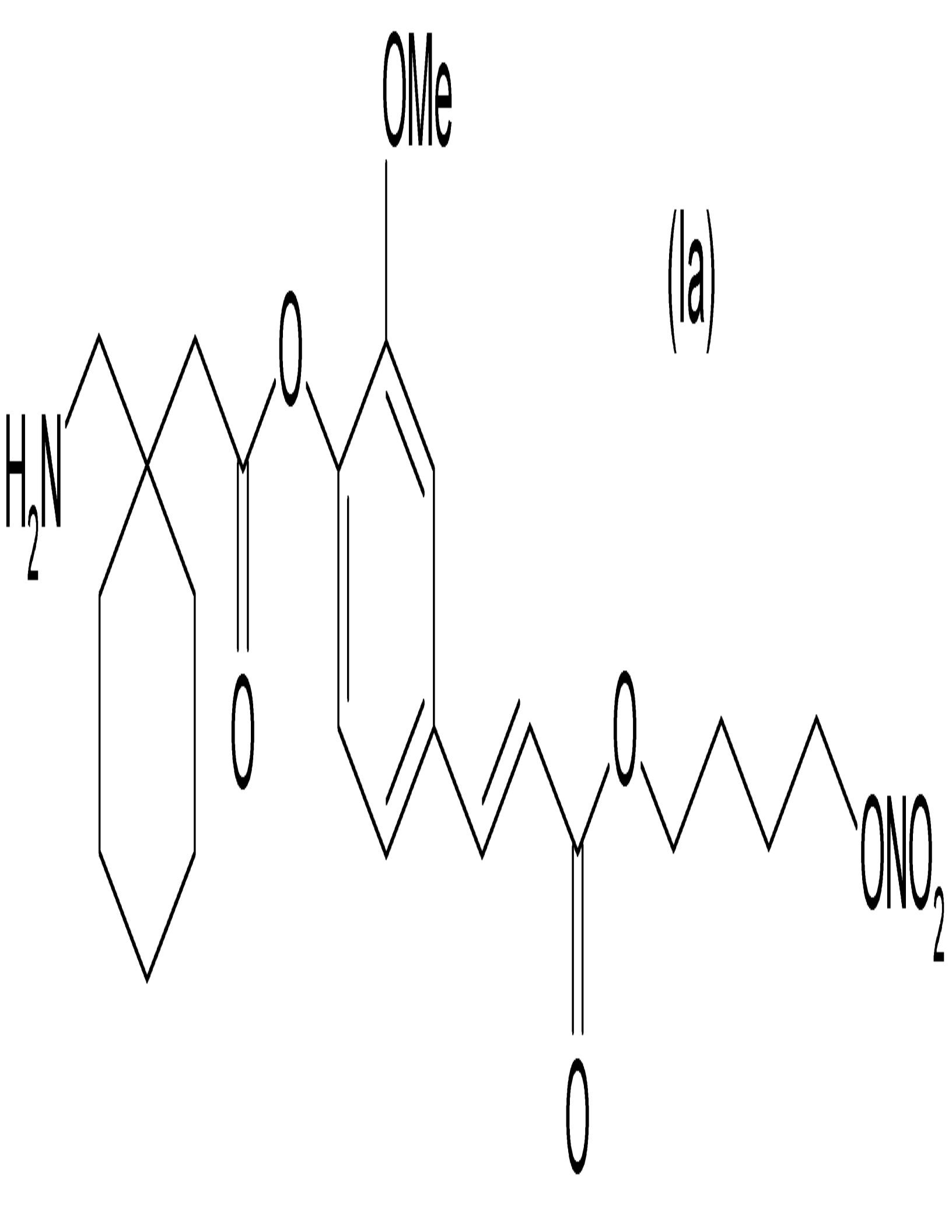
Ry
(i)
—(CH2)n3
—(CH2)n3'
(iii)
(CH2)n3'—O
HOOC
(CH2)n3—
(iv)


OMe
(Ia)
H2N
O
O
O
O
ONO2

DERWENT-ACC-NO: 2003-221389

DERWENT-WEEK: 200560

TITLE: New nitrooxy derivatives used for treating epilepsy

INVENTOR: DEL SOLDATO P; ONGINI E

PATENT-ASSIGNEE: NICOX SA[NICON]

PRIORITY-DATA: 2001IT-MI1307 (June 21, 2001)

PATENT-FAMILY:

PUB-NO	PUB-DATE	LANGUAGE
WO 03000643 A1	January 3, 2003	EN
AU 2002314157 A1	January 8, 2003	EN
IT 1325658 B	December 13, 2004	IT

DESIGNATED-STATES: AE AG AL AU BA BB BG BR BZ CA CN CO CR CU CZ DM DZ EC EE GD GE HR HU ID IL IN IS JP KP KR LC LK LR LT LV MA MG MK MN MX NO NZ OM PH PL RO SG SI SK TN TR TT UA US UZ VN YU ZA AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZM ZW

APPLICATION-DATA:

PUB-NO	APPL-DESCRIPTOR	APPL-NO	APPL-DATE
WO2003000643A1	N/A	2002WO-EP06389	June 11, 2002
IT 1325658B	N/A	2001IT-MI1307	June 21, 2001
AU2002314157A1	Based on	2002AU-314157	June 11, 2002

INT-CL-CURRENT:

TYPE	IPC DATE
CIPS	C07C203/04 20060101
CIPS	C07C229/08 20060101
CIPS	C07C229/28 20060101
CIPS	C07C279/12 20060101
CIPS	C07C279/14 20060101
CIPS	C07C327/34 20060101
CIPS	C07C335/08 20060101
CIPS	C07D213/30 20060101

ABSTRACTED-PUB-NO: WO 03000643 A1

BASIC-ABSTRACT:

NOVELTY - Nitrooxy derivatives (I) are new.

DESCRIPTION - Nitrooxy derivatives of formula A-(B) ba-(C1)ca-NO2 (I) and their salts are new.

ba, ca = 0 or 1 (preferably 1);

A = R-T1;

R = a radical of a precursor drug of formula R2-W(R1)(R0)-(CH2)m;

W = C or N;

R0 = H or (CH2)n-NHR1a;

m, n = 0-2;

R1a = H, C(O)-R1h or C(O)O-R1h;

R1h = U1 or U2;

U1 = 1-10C alkyl, phenyl or benzyl;

U2 = CH(Ry)-NH2, a group of formula (i), C(Ry)(Ry)-OCORy or 1-methyl-1,2,3,6-tetrahydro-pyridin-4yl;

Ry = H or U1;

R1 = H or electronic doublet on the nitrogen atom (free valence);

R2 = U3, U4, U5 or U6, or

R2+R1a+W = 4-10 (preferably 6)C ring;

U3 = phenyl (optionally substituted by halo or at least one OCH3, CF3 or NO2);

U4 = mono- or di-hydroxy substituted benzyl (preferably 3-4 di-hydroxy substituted);

U5 = H2N(C=NH);

U6 = Q-(CH)p3(R8)-(CH)p2(R7)-(C)p1((R6)(R6a)p)-CH(R5)-CH(R4) (where optionally one ethylenic unsaturation is between the C atoms in position 1 and 2, or 3 and 4 or 4 and 5);

p, p1, p2 = 0 or 1;

p3 = 0-10;

R4 = H, 1-6C alkyl or free valence;

R5 = 1-6C alkyl, 3-6C cycloalkyl, free valence or ORa';

Ra' = 1-6C alkyl (optionally substituted by at least one halo (preferably F)) or U3;

R6, R6a, R7, R8 = H, methyl or free valence;

Q = H, OH, ORb', 3-6C cycloalkyl, 1-6C alkyl, H2NC(=NH)NH or H2NC(=S)NH;

Rb' = 1-6C alkyl (optionally substituted by at least one halo (preferably F)), benzyl, or U3;

T1 = (CO)t or (X)t';

X = O, S or NR1c;

R1c = H or 1-5C alkyl;

B = Tb-X2-Tb1;

the precursor compound of B = L-carnosine, anserine, selenocysteine, selenomethionine,

penicillamine, N-acetylpenicillamine, cysteine, N-acetylcysteine, glutathione or their esters (preferably ethyl or isopropyl ester), gallic acid, ferulic acid, gentisic acid, citric acid, caffeic acid, dihydrocaffeic acid, p-cumaric acid, vanillic acid, nordihydroguaiaretic acid, quercetin, catechin, kaempferol, sulfurethyne, ascorbic acid, isoascorbic acid, hydroquinone, gossypol, reductic acid, methoxy hydroquinone, hydroxyhydroquinone, propyl gallate, saccharose, 3,5-di-tertbutyl-4-hydroxy-benzylthio glycolate, p-cumaric alcohol, 4-hydroxy-phenylethylalcohol, coniferyl alcohol, allopurinol, 3,3'-thiodipropionic acid, fumaric acid, dihydroxy maleic acid or edetic acid;

Tb = CO or X;

Tb1 = (CO)tx or (X)txx;

t, t', tx, txx = 0 or 1;

X2 = a bivalent group such that the corresponding of precursor of B has free valences of Tb and Tb1 saturated with OZ, Z or N(ZI)(ZII);

Z, ZI, ZII = H or 1-10 (preferably 1-5)C alkyl;

C1 = Tc-Y;

Tc = CO (when tx = 0) or X (when txx = 0) and ba and ca are 1, or

Tc = CO (when t = 0) or X (when t' = 0), or

Tc = CO (when tx = 0) or X (when txx = 0) and ca = 0, tx = 0 and Tb1 = O;

Y = Yp, Ya or Yar;

Yp = (C)n1x(Rt1x)(Rt1x')-Y3-(C)-n11x(Rt11x)(Rt11x')-O (ii);

n1x = 0-5 (preferably 1);

n11x = 1-5 (preferably 1);

Rt1x, Rt1x', Rt11x, Rt11x' = H or 1-4C alkyl;

Y3 = 5- or 6-membered heterocyclyl containing 1-3 N, O or S heteroatoms;

Ya = R'O or Aa;

Aa = (CH2-CH(ONO2)-CH2-O)nf', (CH2(ONO2)-CH(CH3)-CH2-O)nf', (CH(R1f)-CH2-O)nf or (CH2-CH(R1f)-O)nf;

R1f = H or CH3;

nf' = 1-6 (preferably 1-4);

nf = 1-6 (preferably 2-4);

R' = 1-20 (preferably 2-6)C alkyl or 5-7C cycloalkylene ring (in which at least one carbon atom is substituted by heteroatoms and the ring can have side chains of R' type);

Yar = Yar1 or Yar2;

Yar1 = a group of formula (iii);

Yar2 = a group of formula (iv);

n3 = 0-5, and

n3' = 1-3,

provided that:

(1) ca and ba are not both zero;

(2) when t is 1, t' is 0 and when t' is 1, t is 0;

(3) when tx is 1, then txx is 0 and when tx is 0, then txx is 1;

(4) when W is N , R1 is an electronic doublet on the nitrogen atom (free valence), and

(5) in (ii), when one unsaturation of ethylene type is present, between carbons 1 and 2, R4 and R5 are free valences to form the double bond between carbons 1 and 2; when the unsaturation is between carbons 3 and 4, R6 and R7 are free valences to form the double bond between carbons 3 and 4; when the unsaturation is between carbons 4 and 5, R7 and R8 are free valences to form the double bond between carbons 4 and 5.

None given in the source material.

USE - Used for treating epilepsy (claimed).

ADVANTAGE - (I) Reduce the incidence and the seriousness of convulsive fits with lower side effects, and show improved activity with respect to the precursor drug in the epilepsy treatment. (I) Can be used in an amount of less than the maximum indicated for the precursor drugs and also at a higher doses considering their very good tolerability.

EQUIVALENT-ABSTRACTS:

ORGANIC CHEMISTRY

Preparation: Preparation of (I) comprises e.g. reacting R-COO-Hal with AgNO3 to give R-COO-Y-ONO2 (I').

Preferred Definitions:

Y3 = pyridine having two free valences in the ortho positions with respect to the nitrogen atom, piperazin-1,4-diyl, 1H-pyrazole (3,5-disubstituted), piperidin-1-yl (where the free valence on the ring is in para position to the nitrogen atom);

B = ferulic acid, N-acetylcysteine, cysteine, caffeic acid, hydro-caffeic or gentisic acid;

R = gabapentine, norvaline, arginine, thiocitrulline, pregabaline, (S)3-isobutyl-gamma aminobutyric acid, agmatine, vigabatrine or 2-amino, (3,4-dihydroxyphenyl)propanoic acid (dopa).

Administration is parenteral, oral or topical (claimed).

Administration is optionally in combination with NO donor compounds containing drugs belonging to the classes of aspirin, ibuprofen, paracetamol, naproxen, diclofenac or flurbiprofen.

SPECIFIC COMPOUNDS

16 Compounds (I) are specifically claimed e.g:

1-(aminomethyl)cyclohexane acetic acid 2-methoxy-4-((1E)-3-(4-(nitrooxy)butoxy)-3-oxy-1-porpenyl) phenyl hydrochloride ester (Ia).

To a solution of 1-(aminomethyl)cyclohexanacetic acid (10 g) in mixture of dioxane (100 ml) and water (150 ml), triethylamine (16.27 ml) and di-tert-butyldicarbonate (15.3 g) were added. The reaction mixture was left at room temperature, under stirring for 4 hours and worked up to give 1-(N-tert-butoxycarbonylaminomethyl)cylcohexan acetic acid (A). To a solution of ferulic acid (11.6 g) in tetrahydrofuran (400 ml), tetrabromomethane (39.62 g) and triphenylphosphine (31.34 g) were added. The obtained mixture was kept under stirring at room temperature for 5 hours, filtered, evaporated at reduced pressure and worked up to give 2-methoxy-4-((1E)-3-(4-(bromo)-butoxy)-3-oxy-1-propenyl)phenol. To a solution of this compound (8 g) in acetonitrile (500 ml), silver nitrate (12.25 g) was added. The reaction mixture was heated at 40degreesC for 12 hours sheltered from light and worked up to give 2-methoxy-4-((1E)-3-(4-(nitrooxy) butoxy)-3-oxy-1-propenyl)phenol (C1).

To a solution of (A) (2.5 g) in chloroform (200 ml) and N,N-dimethylformamide (3 ml), (C1) (3.15 g), dicyclohexylcarbodiimide (5.7 g) and N,N-dimethylaminopyridine (33 mg) were added. The reaction mixture was left at room temperature, under stirring for 3 hours and worked up to give 1-(N-tert-butoxycarbonyaminomethyl)cyclohexan acetic acid 2-methoxy-4-((1E)-3-(4-(nitroxy)butoxy)-3-oxy-1-propenyl)phenyl ester.

To a solution of this compound (5 g) in ethyl acetate (100 ml), a solution of 1N HCl in ethyl acetate (50 ml) was added. The reaction mixture was

left overnight at room temperature and concentrated under vacuum and worked up to give 1-(aminomethyl) cyclohexane acetic acid 2-methoxy-4-((1E)-3-(4-(nitrooxy)butoxy)-3-oxy-1-propenyl)phenyl hydrochloride ester (Ia) (1.8 g).

TITLE-TERMS: NEW DERIVATIVE TREAT EPILEPSY

DERWENT-CLASS: B05

CPI-CODES: B06-H; B07-H; B10-A03; B14-J07;

CHEMICAL-CODES: Chemical Indexing M2 *01*
Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G015 G030 G038 G111 G563 H1 H100 H181 H5 H541 H7 H721 H8 J0 J012 J2 J241 J271 K0 K7 K710 M210 M211 M272 M281 M311 M312 M314 M321 M322 M332 M342 M372 M373 M383 M391 M392 M411 M510 M520 M531 M541 M640 M710 P442 Specific Compounds RA9QTR Registry Numbers 673786

Chemical Indexing M2 *02*
Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G012 G030 G038 G111 G563 H1 H100 H181 J0 J011 J2 J241 K0 K7 K710 M280 M311 M323 M342 M372 M373 M391 M392 M411 M510 M520 M531 M541 M640 M710 P442 Specific Compounds RA9QTU Registry Numbers 673789

Chemical Indexing M2 *03*
Fragmentation Code H4 H498 H9 J0 J012 J2 J271 J3 J371 M210 M211 M213 M232 M262 M272 M281 M312 M321

M332 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds RA9R63 Registry Numbers 170395

Chemical Indexing M2 *04* Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J014 J1 J171 J2 J271 J3 J372 M210 M213 M232 M272 M281 M311 M312 M313 M321 M332 M342 M343 M349 M381 M393 M416 M620 M710 P442 Specific Compounds RA9R67 Registry Numbers 96260

Chemical Indexing M2 *05* Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G012 G100 H1 H100 H181 J0 J011 J2 J241 K0 K7 K710 M280 M311 M314 M321 M331 M340 M342 M349 M373 M381 M391 M411 M510 M520 M531 M540 M640 M710 P442 Specific Compounds RA9QTV Registry Numbers 673790

Chemical Indexing M2 *06* Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 H1 H100 H181 J0 J012 J2 J272 J290 J3 J371 J9 K0 K7 K710 M210 M211 M262 M281 M312 M314 M321 M322 M331 M332 M340 M342 M343 M349 M381 M383 M391 M392 M411 M510 M520 M530 M540 M620 M640 M710 P442 Specific Compounds RA9QTX Registry Numbers 673791

Chemical Indexing M2 *07* Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G030 G038 G563 H1 H100 H181 J0 J012 J2

J272 J290 J3 J371 J9 K0 K7 K710 M210 M211 M262 M281 M311 M312 M314 M321 M322 M332 M342 M343 M349 M372 M373 M381 M383 M391 M411 M510 M520 M530 M541 M640 M710 P442 Specific Compounds RA9QTZ Registry Numbers 673795

Chemical Indexing M2 *08* Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 F012 F016 F431 G030 G038 G563 H1 H100 H181 J0 J011 J2 J271 K0 K7 K710 M280 M311 M323 M342 M372 M373 M391 M393 M411 M510 M521 M530 M541 M640 M710 P442 Specific Compounds RA9QU0 Registry Numbers 673797

Chemical Indexing M2 *09* Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G012 G100 H1 H100 H181 J0 J011 J2 J241 K0 K7 K710 L4 L420 M280 M311 M314 M321 M332 M342 M343 M349 M373 M381 M391 M411 M510 M520 M531 M540 M640 M710 P442 Specific Compounds RA9QU1 Registry Numbers 673798

Chemical Indexing M2 *10* Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 H1 H100 H181 J0 J012 J2 J272 J290 J3 J371 J9 K0 K7 K710 L4 L420 M210 M211 M262 M281 M312 M314 M321 M322 M332 M342 M343 M349 M381 M383 M391 M392 M411 M510 M520 M530 M540 M620 M640 M710 P442 Specific Compounds RA9QU3 Registry Numbers 673800

Chemical Indexing M2 *11*
Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G015 G100 H1 H100 H181 H5 H541 H7 H721 H8 J0 J012 J2 J241 J271 K0 K7 K710 L4 L420 M210 M211 M272 M281 M312 M314 M321 M322 M332 M342 M343 M349 M372 M381 M383 M391 M411 M510 M520 M531 M540 M640 M710 P442 Specific Compounds RA9QU4 Registry Numbers 673801

Chemical Indexing M2 *12*
Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G012 G100 H1 H100 H181 J0 J011 J2 J241 K0 K7 K710 L2 L250 M280 M311 M314 M321 M332 M342 M343 M349 M373 M381 M391 M411 M510 M520 M531 M540 M640 M710 P442 Specific Compounds RA9QU5 Registry Numbers 673802

Chemical Indexing M2 *13*
Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G015 G100 H1 H100 H181 H5 H541 H7 H721 H8 J0 J012 J2 J241 J271 K0 K7 K710 L2 L250 M210 M211 M272 M281 M312 M314 M321 M322 M332 M342 M343 M349 M372 M381 M383 M391 M411 M510 M520 M531 M540 M640 M710 P442 Specific Compounds RA9QU6 Registry Numbers 673803

Chemical Indexing M2 *14*
Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 H1

H100 H181 J0 J012 J2 J272 J290 J3 J371 J9 K0 K7 K710 L2 L250 M210 M211 M262 M281 M312 M314 M321 M322 M332 M342 M343 M349 M381 M383 M391 M392 M411 M510 M520 M530 M540 M620 M640 M710 P442 Specific Compounds RA9QU7 Registry Numbers 673804

Chemical Indexing M2 *15* Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G012 G100 J0 J011 J3 J331 K0 K7 K710 L2 L250 M280 M311 M314 M321 M332 M342 M373 M383 M391 M411 M510 M520 M531 M540 M640 M710 P442 Specific Compounds RA9QU8 Registry Numbers 673805

Chemical Indexing M2 *16* Fragmentation Code C116 F010 F011 F012 F014 F015 F020 F021 F140 F432 G001 G003 G010 G011 G012 G013 G015 G019 G050 G100 G111 G112 G113 G553 G563 H100 H101 H102 H103 H141 H181 H182 H201 H321 H341 H402 H442 H541 H600 H641 H642 H643 H685 H721 J011 J012 J013 J231 J271 J311 J331 J371 J5 J521 J581 J582 K351 K352 K353 K620 K640 K699 K710 K810 K830 K850 K899 L250 L410 L463 L640 L660 L699 L922 M121 M123 M129 M132 M135 M150 M210 M211 M212 M213 M214 M215 M216 M220 M221 M222 M223 M224 M225 M226 M231 M232 M233 M240 M262 M271 M272 M273 M280 M281 M282 M283 M311 M312 M313 M314 M315 M316 M320 M321 M322 M323 M331 M332 M333 M334 M340 M342 M343 M344 M349 M353 M371 M372 M373

M381 M382 M383 M391 M392 M393 M413 M414 M415 M416 M510 M520 M521 M522 M530 M531 M532 M533 M540 M541 M620 M630 M640 M650 M710 P442 Markush Compounds 008706801

Chemical Indexing M2 *17* Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J014 J1 J171 J2 J271 J3 J372 M210 M213 M232 M272 M281 M311 M312 M313 M321 M332 M342 M343 M349 M381 M393 M416 M620 M710 P442 Specific Compounds RA9R66 Registry Numbers 674340

Chemical Indexing M2 *18* Fragmentation Code F011 F015 F521 H1 H100 H182 H2 H201 J0 J012 J1 J171 J3 J371 M210 M211 M273 M281 M312 M322 M332 M342 M343 M349 M371 M381 M391 M413 M510 M521 M530 M540 M710 M800 P442 Specific Compounds R11742 Registry Numbers 87509

Chemical Indexing M2 *19* Fragmentation Code B434 H1 H100 H181 H4 H498 H9 J0 J011 J1 J171 M280 M312 M321 M332 M343 M349 M381 M391 M411 M510 M520 M530 M540 M620 M710 P442 Specific Compounds R07941 Registry Numbers 125177

Chemical Indexing M2 *20* Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J011 J1 J171 M280 M314 M321 M333 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds R00064 R22037 Registry Numbers

8198

Chemical Indexing M2 *21*
Fragmentation Code F011 F015 F521 H1 H100 H182 H2 H201 J0 J012 J2 J271 J3 J371 M210 M211 M212 M272 M273 M281 M312 M322 M332 M342 M343 M349 M371 M381 M391 M413 M510 M521 M530 M540 M710 P442 Specific Compounds RA9R5N Registry Numbers 674321

Chemical Indexing M2 *22*
Fragmentation Code B434 H1 H100 H181 H5 H598 H9 J0 J011 J1 J171 M210 M211 M271 M281 M313 M321 M332 M343 M349 M381 M391 M411 M510 M520 M530 M540 M620 M710 P442 Specific Compounds R06089 Registry Numbers 106864

Chemical Indexing M2 *23*
Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J011 J1 J171 M280 M312 M321 M332 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds R01628 R12616 Registry Numbers 132396 141452 188253 2466 8188

Chemical Indexing M2 *24*
Fragmentation Code H4 H498 H9 J0 J012 J1 J171 J3 J371 M210 M211 M262 M281 M312 M321 M332 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds R04369 Registry Numbers 12143

Chemical Indexing M2 *25*

Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J014 J1 J172 J3 J372 M280 M311 M312 M313 M321 M332 M342 M343 M349 M381 M393 M416 M620 M710 P442 Specific Compounds R00297 Registry Numbers 882

Chemical Indexing M2 *26* Fragmentation Code G013 G100 H4 H401 H441 H7 H721 H8 J0 J011 J1 J171 M280 M312 M321 M332 M342 M372 M391 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R01664 Registry Numbers 91684

Chemical Indexing M2 *27* Fragmentation Code G015 G100 H4 H401 H441 H5 H541 H8 J0 J011 J1 J131 M210 M211 M272 M281 M320 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R01012 Registry Numbers 110027

Chemical Indexing M2 *28* Fragmentation Code G015 G100 H4 H402 H442 H8 J0 J011 J1 J171 M280 M312 M321 M332 M342 M372 M391 M414 M510 M520 M531 M540 M710 P442 Specific Compounds RA03BO Registry Numbers 93147

Chemical Indexing M2 *29* Fragmentation Code G015 G100 H4 H402 H442 H7 H721 H8 J0 J011 J1 J171 M280 M312 M321 M332 M342 M372 M391 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R11260 Registry Numbers 89783

Chemical Indexing M2 *30*
Fragmentation Code H4 H401 H481 H8 J0 J013 J1 J173 M280 M313 M321 M332 M344 M349 M381 M391 M416 M620 M710 P442 Specific Compounds R00419 R07029 Registry Numbers 104520 129792 129991 130395 132222 133510 140723 140725 159060 191428 2471 250717 278358 278359 3589 849 87079 95073 95095 99996

Chemical Indexing M2 *31*
Fragmentation Code G015 G100 H4 H402 H442 H8 J0 J011 J1 J131 M280 M320 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R01283 Registry Numbers 96020

Chemical Indexing M2 *32*
Fragmentation Code G015 G100 H4 H401 H441 H5 H541 H7 H721 H8 J0 J011 J1 J171 M210 M211 M272 M281 M312 M321 M332 M342 M372 M391 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R13076 Registry Numbers 95106

Chemical Indexing M2 *33*
Fragmentation Code G017 G100 H4 H403 H443 H8 J0 J011 J1 J131 M280 M320 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R01170 R09472 Registry Numbers 7650

Chemical Indexing M2 *34*
Fragmentation Code G015 G019 G100 H4 H404 H444 H8 M1 M121 M135 M280

M315 M321 M333 M342 M414 M510 M520 M532 M540 M710 P442 Specific Compounds R06755 Registry Numbers 102281

Chemical Indexing M2 *35* Fragmentation Code D014 D023 D120 G015 G100 H4 H404 H405 H421 H444 H8 J5 J521 J522 L9 L960 M1 M113 M280 M320 M412 M511 M520 M531 M540 M710 P442 Specific Compounds R00971 RA0055 Registry Numbers 105172 129528

Chemical Indexing M2 *36* Fragmentation Code D013 D023 D120 G015 G100 H4 H405 H421 H444 H8 M1 M113 M280 M320 M412 M511 M520 M531 M540 M710 P442 Specific Compounds R04686 Registry Numbers 90953

Chemical Indexing M2 *37* Fragmentation Code D014 D023 D120 G013 G100 H4 H403 H443 H8 J5 J522 L9 L960 M1 M113 M280 M320 M412 M511 M520 M531 M540 M710 P442 Specific Compounds R08510 Registry Numbers 21764

Chemical Indexing M2 *38* Fragmentation Code F012 F013 F014 F015 F113 H4 H403 H421 H482 H8 J5 J522 K0 L8 L818 L821 L832 L9 L942 L960 M280 M312 M321 M332 M343 M373 M391 M413 M510 M521 M530 M540 M710 P442 Specific Compounds R00035 R04454 Registry Numbers 185

Chemical Indexing M2 *39*
Fragmentation Code F012 F013 F014 F015 F017 F113 H4 H403 H421 H482 H8 J5 J522 K0 L8 L818 L821 L832 L9 L942 L960 M280 M312 M321 M332 M343 M373 M391 M413 M510 M521 M530 M540 M710 P442 Specific Compounds R06288 R16366 Registry Numbers 98195

Chemical Indexing M2 *40*
Fragmentation Code G013 G100 H4 H402 H442 H8 M280 M320 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R01041 Registry Numbers 58

Chemical Indexing M2 *41*
Fragmentation Code G023 G024 G029 G221 G299 H4 H405 H444 H8 J4 J432 M1 M114 M210 M211 M213 M232 M240 M283 M320 M414 M510 M520 M532 M540 M710 P442 Specific Compounds R11378 Registry Numbers 96388

Chemical Indexing M2 *42*
Fragmentation Code G036 G552 H4 H402 H462 H8 J5 J561 M280 M320 M415 M510 M520 M530 M541 M710 P442 Specific Compounds RA1YBQ Registry Numbers 294262

Chemical Indexing M2 *43*
Fragmentation Code G015 G100 H4 H402 H442 H5 H541 H8 M210 M211 M272 M281 M320 M414 M510 M520 M531 M540 M710 P442 Specific Compounds RA056K Registry Numbers 19087

Chemical Indexing M2 *44*
Fragmentation Code G015 G100 H4 H403 H443 H8 M280 M320 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R08208 Registry Numbers 23884

Chemical Indexing M2 *45*
Fragmentation Code G017 G100 H4 H403 H443 H8 J0 J011 J2 J231 M210 M213 M231 M272 M281 M320 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R04639 Registry Numbers 95847

Chemical Indexing M2 *46*
Fragmentation Code F012 F013 F014 F015 F016 F017 F019 F113 F123 H4 H405 H424 H483 H5 H521 H8 K0 L8 L814 L818 L822 L831 M1 M126 M141 M280 M311 M323 M342 M373 M393 M413 M510 M522 M530 M540 M710 P442 Specific Compounds R00135 Registry Numbers 133509 2853

Chemical Indexing M2 *47*
Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G030 G038 G563 H1 H100 H181 J0 J011 J2 J271 K0 K7 K710 M280 M311 M314 M321 M322 M332 M342 M372 M373 M383 M391 M411 M510 M520 M530 M541 M640 M710 P442 Specific Compounds RA9QUA Registry Numbers 673807

Chemical Indexing M2 *48*
Fragmentation Code G013 G100 H4

H402 H441 H481 H7 H721 H8 M280 M313 M321 M332 M342 M373 M391 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R11985 Registry Numbers 141069

Chemical Indexing M2 *49* Fragmentation Code G015 G100 H4 H402 H441 H481 H5 H541 H7 H721 H8 M210 M211 M272 M281 M313 M321 M332 M342 M373 M391 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R14887 Registry Numbers 8315

Chemical Indexing M2 *50* Fragmentation Code G013 G100 H4 H402 H441 H481 H8 M280 M312 M321 M332 M342 M373 M391 M414 M510 M520 M531 M540 M710 P442 Specific Compounds R14354 Registry Numbers 9344

Chemical Indexing M2 *51* Fragmentation Code D011 D920 J5 J521 L9 L941 M280 M320 M412 M511 M520 M530 M540 M710 P442 Ring Index Numbers 01174 Specific Compounds R01218 R04867 Registry Numbers 86977

Chemical Indexing M2 *52* Fragmentation Code H5 H598 H9 J0 J012 J1 J172 M280 M312 M322 M332 M342 M381 M392 M416 M620 M710 P442 Specific Compounds R05349 Registry Numbers 108778

Chemical Indexing M2 *53*

Fragmentation Code H4 H401 H481 H8 J0 J012 J1 J172 J5 J581 K0 L5 L560 M280 M311 M321 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds R13040 Registry Numbers 69951

Chemical Indexing M2 *54* Fragmentation Code H7 H721 J0 J012 J1 J172 M280 M312 M321 M332 M342 M382 M391 M416 M710 P442 Specific Compounds R00902 R04891 Registry Numbers 130347 132553 134096 134238 143998 205770 205776 232427 7658

Chemical Indexing M2 *55* Fragmentation Code C017 C100 C800 C801 C803 C804 C805 C806 C807 G015 G100 H5 H541 H7 H721 H8 J0 J012 J2 J241 J3 J371 K0 K7 K710 L2 L250 M210 M211 M272 M281 M312 M313 M314 M321 M332 M342 M372 M381 M383 M391 M411 M510 M520 M531 M540 M640 M710 P442 Specific Compounds RA9QUB Registry Numbers 673808

Chemical Indexing M2 *56* Fragmentation Code G017 G100 H4 H401 H441 H498 H8 H9 J0 J011 J2 J271 M210 M214 M233 M240 M282 M311 M322 M342 M349 M373 M381 M391 M414 M510 M520 M531 M540 M710 P442 Specific Compounds RA9R5G Registry Numbers 674315

Chemical Indexing M2 *57* Fragmentation Code F014 F521 H1

H100 H181 J0 J012 J2 J271 J3 J371 M210 M212 M272 M281 M312 M322 M332 M342 M343 M349 M371 M381 M391 M413 M510 M521 M530 M540 M710 P442 Specific Compounds RA9R5J Registry Numbers 674317

Chemical Indexing M2 *58* Fragmentation Code F014 F521 H1 H100 H181 J0 J012 J2 J271 J3 J371 M210 M213 M232 M272 M281 M312 M322 M332 M342 M343 M349 M371 M381 M391 M413 M510 M521 M530 M540 M710 P442 Specific Compounds RA9R5K Registry Numbers 674318

Chemical Indexing M2 *59* Fragmentation Code F011 F015 F521 H1 H100 H182 H2 H201 J0 J012 J2 J271 J3 J371 M210 M211 M213 M232 M272 M273 M281 M312 M322 M332 M342 M343 M349 M371 M381 M391 M413 M510 M521 M530 M540 M710 P442 Specific Compounds RA9R5O Registry Numbers 674322

Chemical Indexing M2 *60* Fragmentation Code B434 H1 H100 H181 H4 H498 H9 J0 J011 J2 J271 M210 M212 M272 M281 M312 M321 M332 M343 M349 M381 M391 M411 M510 M520 M530 M540 M620 M710 P442 Specific Compounds RA9R5R Registry Numbers 674325

Chemical Indexing M2 *61* Fragmentation Code B434 H1 H100 H181 H4 H498 H9 J0 J011 J2 J271

M210 M213 M232 M272 M281 M312 M321 M332 M343 M349 M381 M391 M411 M510 M520 M530 M540 M620 M710 P442 Specific Compounds RA9R5S Registry Numbers 674327

Chemical Indexing M2 *62* Fragmentation Code B434 H1 H100 H181 H5 H598 H9 J0 J011 J2 J271 M210 M211 M212 M271 M272 M281 M313 M321 M332 M343 M349 M381 M391 M411 M510 M520 M530 M540 M620 M710 P442 Specific Compounds RA9R5U Registry Numbers 674329

Chemical Indexing M2 *63* Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J011 J2 J271 M210 M212 M272 M281 M314 M321 M333 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds RA9R5Y Registry Numbers 674704

Chemical Indexing M2 *64* Fragmentation Code B434 H1 H100 H181 H5 H598 H9 J0 J011 J2 J271 M210 M211 M213 M232 M271 M272 M281 M313 M321 M332 M343 M349 M381 M391 M411 M510 M520 M530 M540 M620 M710 P442 Specific Compounds RA9R5W Registry Numbers 674331

Chemical Indexing M2 *65* Fragmentation Code H4 H498 H9 J0 J012 J2 J271 J3 J371 M210 M211 M212 M262 M272 M281 M314 M321 M333 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds RA9R60

Registry Numbers 674706

Chemical Indexing M2 *66*
Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J011 J2 J271 M210 M213 M232 M272 M281 M314 M321 M333 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds RA9R5Z Registry Numbers 674334

Chemical Indexing M2 *67*
Fragmentation Code H4 H498 H9 J0 J012 J2 J271 J3 J371 M210 M211 M212 M262 M272 M281 M312 M321 M332 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds RA4DPH Registry Numbers 411706

Chemical Indexing M2 *68*
Fragmentation Code H4 H498 H9 J0 J012 J1 J171 J3 J371 M210 M211 M262 M281 M314 M321 M333 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds RA24WX Registry Numbers 86396

Chemical Indexing M2 *69*
Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J011 J2 J271 M210 M213 M232 M272 M281 M312 M321 M332 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds RA5ZNK Registry Numbers 92121

Chemical Indexing M2 *70*
Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J011 J2 J271 M210 M212 M272 M281 M312 M321 M332 M343 M349

M381 M391 M416 M620 M710 P442 Specific Compounds RA30IJ Registry Numbers 92120

Chemical Indexing M2 *71* Fragmentation Code H1 H103 H182 J0 J014 J1 J173 M280 M311 M312 M321 M323 M332 M342 M349 M381 M383 M391 M393 M416 M620 M710 P442 Specific Compounds R00195 R04870 Registry Numbers 129933 130071 130946 131585 132742 133268 3330 4238 5021 591 93951 93962

Chemical Indexing M2 *72* Fragmentation Code H4 H498 H9 J0 J012 J2 J271 J3 J371 M210 M211 M213 M232 M262 M272 M281 M314 M321 M333 M343 M349 M381 M391 M416 M620 M710 P442 Specific Compounds RA9R61 Registry Numbers 674336

Chemical Indexing M2 *73* Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J014 J1 J171 J2 J271 J3 J372 M210 M212 M272 M281 M311 M312 M313 M321 M332 M342 M343 M349 M381 M393 M416 M620 M710 P442 Specific Compounds RA9R65 Registry Numbers 674339

Chemical Indexing M2 *74* Fragmentation Code H1 H100 H181 H4 H498 H9 J0 J014 J1 J171 J2 J271 J3 J372 M210 M212 M272 M281 M311 M312 M313 M321 M332 M342 M343 M349 M381 M393 M416 M620 M710 P442 Specific Compounds RA3ITX Registry Numbers

96259

Chemical Indexing M2 *75*
Fragmentation Code F014 F521 H1
H100 H181 J0 J012 J1 J171 J3 J371
M280 M312 M322 M332 M342 M343 M349
M371 M381 M391 M413 M510 M521 M530
M540 M710 P442 Specific Compounds
R08807 Registry Numbers 90096

UNLINKED-DERWENT-REGISTRY-NUMBERS: ; 0035U ; 0035S ;
0064U ; 0064S ;
0135U ; 0135S ;
0195U ; 0195S ;
0297U ; 0297S ;
0419U ; 0419S ;
0902U ; 0902S ;
0971U ; 0971S ;
1012U ; 1012S ;
1041U ; 1041S ;
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